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DEPARTMENT OF COMMERCE

National Institute of Standards and Technology

[Docket Number: 230710-0163]

Request for Information Regarding File Specification for Findable, Accessible, Interoperable, and Reusable (FAIR) Containerized Computational Software (FAIR-CCS)

AGENCY: National Institute of Standards and Technology, Department of Commerce.

ACTION: Notice of public meetings; request for information.

SUMMARY: The National Institute of Standards and Technology (NIST) is evaluating and improving the specification for achieving interoperability of containerized computational software. Adherence to a specification for *Findable*, *Accessible*, *Interoperable*, and *Reusable (FAIR)* Containerized Computational Software (FAIR-CCS) enables better reuse of containerized tools in complex data analyses by chaining tools into computational workflows. NIST requests information from the community on approaches to achieving interoperability of containerized software, designing a container manifest file that meets the community needs, and lowering the barrier for constructing such a manifest file. Responses to this RFI will also inform a possible revision of the current approach to achieving FAIR-CCS via a manifest file, the entries in the current manifest file specification of FAIR-CCS, and the current tools that aim at automating adherence to the FAIR-CCS manifest specification. NIST will host a workshop on FAIR-CCS at the times and location indicated below and will discuss the responses to this RFI at the workshop.

DATES:

For Comments:

Comments in response to this RFI must be received by 5:00 PM Eastern time on December 7, 2023. Written comments in response to the RFI should be submitted according to the instructions in the **ADDRESSES** and **SUPPLEMENTARY INFORMATION** sections below. Submissions received after that date may not be considered.

For Public Meetings/Webcast:

A virtual meeting will be held on December 5-7, 2023 from 11 a.m. to 3 p.m. Eastern Time. Requests to participate must be received via the virtual meeting website no later than December 1, 2023.

ADDRESSES:

For Comments:

Responses can be submitted by either of the following methods:

- *Electronic submission:* Submit electronic public comments via the Federal e-Rulemaking Portal.

  1. Go to *www.regulations.gov* and enter [NIST-2023-0003] in the search field,
  2. Click the "Comment Now!" icon, complete the required fields, and
  3. Enter or attach your comments.

- E-mail: Comments in electronic form may also be sent to wipp-team@nist.gov. Include "RFI Response: FAIR-CCS" in the subject line of the message.

Instructions: Attachments will be accepted in plain text, Microsoft Word, or Adobe PDF formats. Comments containing references, studies, research, and other empirical data that are not widely published should include copies or electronic links of the referenced materials.

All comments responding to this document will be a matter of public record. Relevant comments will generally be available on the Federal eRulemaking Portal at https://www.Regulations.gov and, after the comment period closes, on NIST's website at

https://www.nist.gov/news-events/events/2023/12/2nd-international-workshop-fair-containerized-computational-software. NIST will not accept comments accompanied by a request that part or all of the material be treated confidentially because of its business proprietary nature or for any other reason. Therefore, do not submit confidential business information or otherwise sensitive, protected, or personal information, such as account numbers, Social Security numbers, or names of other individuals

For Public Meetings/Webcast:

A December 5-7, 2023 public meeting will be held virtually by NIST.

Details about attending the meeting and accessing the video webcast are available at https://www.nist.gov/news-events/events/2023/12/2nd-international-workshop-fair-containerized-computational-software.

FOR FURTHER INFORMATION CONTACT: Dr. Peter Bajcsy, Project Lead, Software and Systems Division, Information Technology Laboratory, National Institute of Standards and Technology, 100 Bureau Drive MS 2201, Gaithersburg, MD 20899, 301-975-2958, or by email to peter.bajcsy@nist.gov.

SUPPLEMENTARY INFORMATION:

Background

A virtual software container consists of a package of software code with all of the required elements to run regardless of the environment. For example, containers for a containerized application include all of the application's system libraries and configuration files and can run on any host operating system. This process, known as containerization, ensures that applications are portable, scalable, and distributed more efficiently.

The usage of software containers has been around for decades but has gained more popularity within the last ten years. With this increasing popularity of software containers as standardized units for deployment, research communities have adopted the practice of

containerizing diverse software components such as algorithms, tools, or modules to run on institutional or commercially available computer cluster, cloud, or high-performance computing (HPC) resources, because running software containers on these platforms provides more opportunity for scalability with minimum resource usage. For example, in biomedical microscopy imaging, stakeholders cope with very large datasets as the advancements in microscope designs and automated acquisition generate terabyte-size image collections in a relative short time span.

Stakeholders also strive to reuse containerized tools and reproduce complex workflow analyses through container-based workflows to improve researchers reproducibility of research processes to increase efficiency, reliability, and collaboration. Accordingly, there is an opportunity in biomedical microscopy imaging to improve the reuse and reproducibility of analyses via specifications of interoperable containerized algorithms (i.e., computational tools or software plugins) in order to create these container-based workflows (i.e., chained containerized algorithms).

Given the complex analyses in working with software containers, heterogeneous file formats and storage mechanisms, a variety of scientific workflow engines, distributed computational and storage environments, and application programming interfaces to metadata registries and ontologies, the stakeholders are expected to be from academia, industry, and government.

Public Meetings

A public meeting will be held on December 5-7, 2023 as indicated in the **DATES** and **ADDRESSES** section. Requests to participate must be received via the meeting website at https://www.nist.gov/news-events/events/2023/12/2nd-international-workshop-fair-containerized-computational-software by December 1, 2023.

Request for Information

Respondents are encouraged – but are not required – to respond to each topic area and to present their responses after each topic area. The following topic areas cover the major areas about which NIST seeks comment. Respondents may organize their submissions in response to this RFI in any manner. Responses may include estimates, which should be identified as such.

All relevant responses that comply with the requirements listed in the **DATES** and **ADDRESSES** sections of this RFI will be considered**.**

NIST is requesting information related to the following topics:

1) Approaches to chain containerized computational software
2) Important characteristics of sets of containerized computational software for reuse
3) Methods to facilitate the characterization of containerized computational software
4) Best practices for containerization of computational algorithms and for the interfaces between containerized algorithms accessing datasets in heterogeneous storage environments
5) Best practices for finding containerized software tools and container-based workflows in online registries using application programming interfaces (APIs)
6) Best practices for executing container-based workflows using workflow engines and job schedulers for computational resource management in distributed computational environments

Authority: 15 U.S.C. 272(b) & (c); 15 U.S.C. 278g-3.

Alicia Chambers,

NIST Executive Secretariat.

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